Heavy Quark Fragmentation at NNLO:

from LEP to the Tevatron and LHC

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Work in progress with:

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Outline

1) Introduction: b- production at hadron colliders

- Importance at the Tevatron and LHC
- Theoretical uncertainties: how can we improve on them?
- The role of Fragmentation Functions (FF).

2) How to extract b-FF's with NNLO accuracy?

New level of perturbative input needed:

- All about the three-loop splitting functions in QCD
- Perturbative challenges: calculations in Mellin space
- b-fragmentation in e+e- at NNLO (two loops): extraction of FF's

3) Future challenges and potential applications.

Motivation

Study of all processes at hadron colliders require pdf's.

Why? Because they give the connection between QCD partons and the physical identified hadrons (the proton).

Precise knowledge of pdf's needed:

- they represent an irreducible uncertainty in all observables

➔ improving only the perturbative description of an observable beyond the accuracy of the pdf's does not make sense.

The same applies for FF's in processes where specific hadrons are identified or, in general, to observables sensitive to collinear radiation (single-particle etc.)

Pdf's	FF's
- Space-like DGLAP evolution	- Time-like DGLAP evolution
- Known to NNLO	- Known to NLO + ns NNLO
-Curci, Furmanski, Petronzio (1980)	- Curci, Furmanski, Petronzio (1980)
- Moch, Vermaseren, Vogt (2004)	- A.M., Moch, Vogt (2006)

Motivation

- I'll be interested only in b-quark production and fragmentation (applicable in principle also for charm – more later),

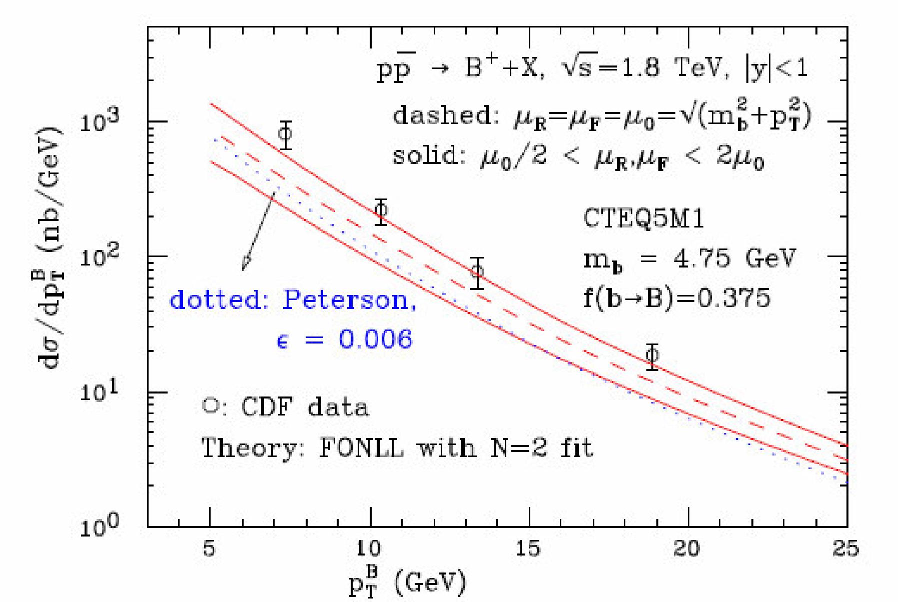
- Important observable! Many b's produced at LEP, HERA, Tevatron; especially LHC and ILC.

Recall the b-production saga at the Tevatron:

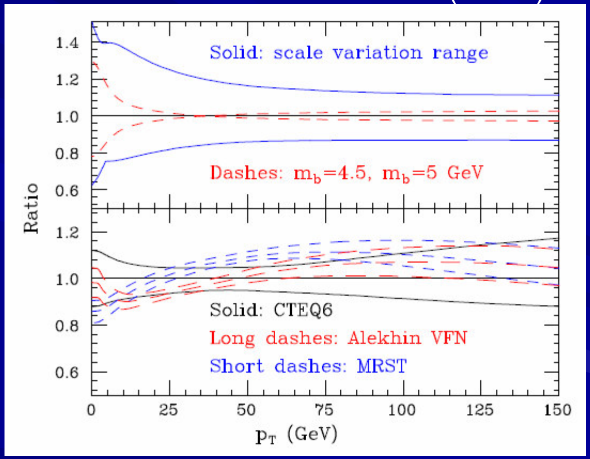
Conclusion: theoretically correct, NLO-level modeling, decreased the discrepancy between theory and experiment:

" A full calculation of next-to-next-to-leading QCD contributions, years ahead in the future, might finally also contribute to explain the apparent discrepancy "

Cacciari, Nason (2002)



Cacciari et al. (2003)



At large PT the theory uncertainty in excess of 20%.

Motivation

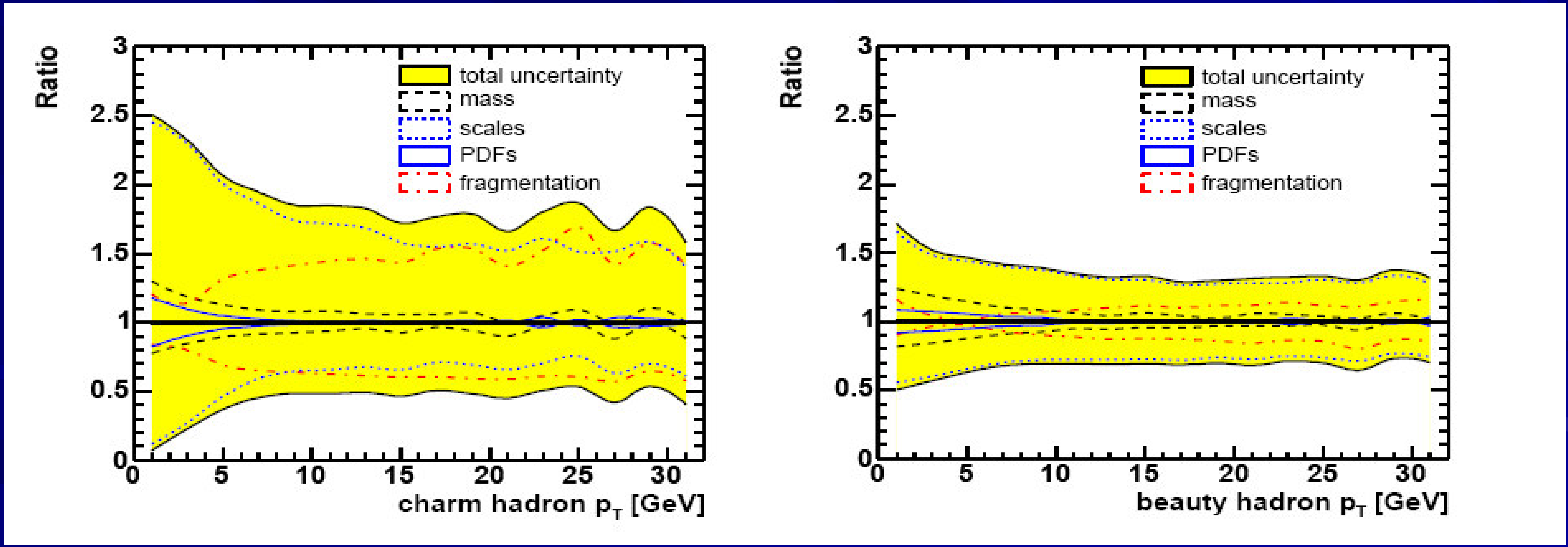
Heavy flavor production at the LHC:

- huge number of b-quarks: ~100,000/sec
- much larger P_T accessible compared to the Tevatron ~ 1000 GeV
- great experimental studies of b-quark P_T - spectra possible:

  16M selected B-events/year at CMS alone.

How can theory meet this challenge?

Here are the theoretical uncertainties at LHC (HERA-LHC working group hep-ph/0601164):



Heavy flavor fragmentation is a dominant uncertainty!

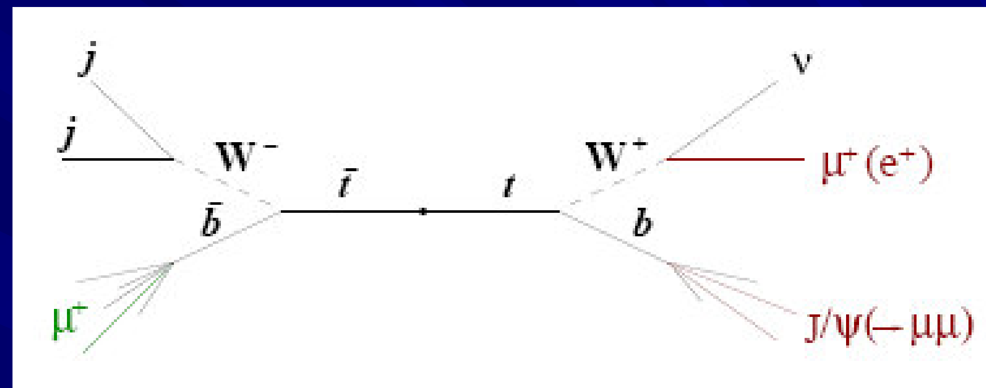
Motivation

b-quark P_T - spectra are not the only interesting physics sensitive to non-perturbative fragmentation.

Top mass measurement from b-fragmentation:

$$\Delta m_{top} \leq 1.5\mathrm{GeV}$$

$$\Delta m_{top}^{exp} \approx 0.5\mathrm{GeV}$$



- Method proposed by A. Kharchilava, hep-ph/9912320.
- Further studies with MC's:
  Corcella, Mangano and Seymour: hep-ph/0004179
- Based on HERWIG 6.0 and 6.1
- Detailed study from CMS (2006): … only after the first year or so the dominant uncertainty will be systematical which in turn is dominated by theory… (N)NLO will be needed…

The largest irreducible uncertainty is from b-fragmentation.

A set of fragmentation functions at NNLO is needed.

Motivation: summary

What is needed to get Fragmentation Functions at NNLO?

From the factorization Theorem:

Predicted for hadron colliders → $$\frac{d\sigma_B}{dp_T} = \frac{d\sigma_b}{dp_T} \otimes D^{DGLAP} \otimes D^{ini} \otimes D^{\text{n.p.}}_{b\to B}$$

Measured at e^+e^- → $$\frac{d\sigma_B}{dE} = \frac{d\sigma_b}{dE} \otimes D^{DGLAP} \otimes D^{ini} \otimes D^{\text{n.p.}}_{b\to B}$$

Physical intuition about heavy flavor production:

1. partons are produced at large scale Q>>m in the hard scattering (→massless),
2. they subsequently perturbatively evolve down to scales O(m) (DGLAP),
3. we assume that B-flavored meson results from the non-perturbative transition b → B, i.e. initiated by a b-quark.
4. however a b-quark can result from the perturbative splitting of other flavors at the scale ~ m (Dini).

Motivation: summary

What is needed to get Fragmentation Functions at NNLO?

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- e^+e^- coefficient functions at two loops Known and checked:

  Rijken, van Neerven (1996),
  A.M., S-O. Moch (2006)

- DGLAP evolution: three-loop (NNLO) time like splitting functions
  Needed for NNLL resummation of large collinear logs $\ln(P_T/m)$ or $\ln(Q/m)$

  Non-singlets available:
  A.M., S-O. Moch, A. Vogt (2006)

- Perturbative fragmentation functions at NNLO All components known:
  Kirill Melnikov, A.M.; A.M. (2004)

- Fit to the LEP data of b- energy spectra In progress … with M. Cacciari, S-O. Moch

Perturbative components

Derivation of the 3-loop (NNLO) time-like splitting functions.

Idea: extract them from the $1/\epsilon$ pole of any collinearly sensitive observable.

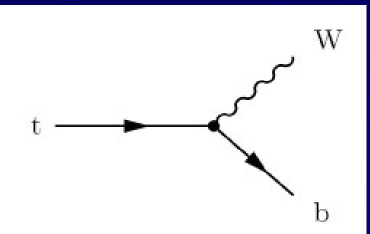
This is well known, but just for completeness, let me mention how that works…

Example:

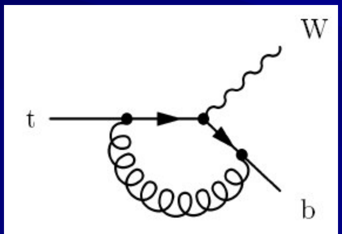
Process: top-decay to massless b-quark $t \to b + X$

Observable: the energy spectrum of the b-quarks.

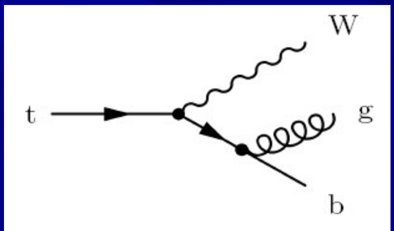
This is an inclusive observable and we include unresolved real radiation too.



Born-level process



1-loop virtual correction



Single gluon radiation

After UV renormalization, the soft singularities cancel but there are remaining collinear singularities …

Up to NLO, this observable takes the form:

$$\frac{d\Gamma}{dz} = \delta(1-z) + \alpha_s \left(\frac{P^{(0)}(z)}{\epsilon} + C(z) + O(\epsilon) \right) + O(\alpha_s^2)$$

Perturbative components

The general situation in the massless case:

$$\frac{d\sigma_a}{dz}(z,Q,\epsilon) = \sum_b \frac{d\hat{\sigma}_b}{dz}(z,Q,\mu) \otimes \Gamma_{ba}(z,\mu,\epsilon)$$

$$\Gamma_{ba} = \delta_{ab}\delta(1-z) - \left(\frac{\alpha_s}{2\pi}\right)\frac{P^{(0)}_{ab}(z)}{\epsilon} + \left(\frac{\alpha_s}{2\pi}\right)^2\left[\frac{1}{2\epsilon^2}\left(P^{(0)}_{ac}\otimes P^{(0)}_{cb}(z) + \beta_0 P^{(0)}_{ab}(z)\right) - \frac{1}{2\epsilon}P^{(1)}_{ab}(z)\right]$$

Two approaches:

1) use specific process (like e^+e^-):
- more complicated to evaluate
- can produce the coefficient functions too (the terms of ϵ^0)
- added bonus: precise determination of the strong coupling from Longitudinal fragmentation.

2) process-independent evaluation in a fictitious process (with L. Dixon):
- simpler to compute, but
- no additional benefit beyond the splitting functions
- related approaches used previously at two loops:

Kosower, Uwer (2001)

Melnikov, A.M.; A.M. (2004)

- what happens at 3-loops? Very hard IBP reductions; very slow with Laporta. Seems unfeasible in momentum (z-) space.

Perturbative components

A side remark: what are "IBP reductions" and "Laporta" anyway?

A 3 slide introduction to the current state of the art technique for higher order calculations.

Consider the following Feynman integral:

$$I(p^2,d) = \int d^dk \frac{2p.k}{k^2(p-k)^2}$$

← Looks messy, especially at higher loops (and legs).

Let's choose better notations:

- there are only two invariants → introduce the two propagators:

$$P_1 = k^2 \ ; \ P_2 = (p-k)^2$$

and

$$B(n_1,n_2) = \int d^dk \frac{1}{P_1^{n_1} P_2^{n_2}}$$

Then we can rewrite the desired integral as:

$$I = p^2 B(1,1) + B(0,1) - B(1,0)$$

In general:

$$I(p^2, z, \dots) = \sum_{n_1,\dots,n_k} C_{n_1,\dots,n_k} B(n_1,\dots,n_k)$$

Perturbative components

A side remark: what are “IBP reductions” and “Laporta” anyway?

The big step: The integrals B(…) are not independent on each other!

Consider the following “Integration by Parts” Identity (IBP):

Chetyrkin, Tkachov (1981)

$$0 = \int d^d k \frac{d}{dk_\mu} \left(p^\mu \frac{1}{k^2 (p-k)^2} \right)$$

If we work it out we get:

$$B(2,0) = B(0,2) + p^2 \left[\ B(2,1) - B(1,2)\ \right]$$

Therefore, not all B’s are independent!

The outcome:

- in realistic problems we encounter 1,000 – 100,000 … B’s
- only dozens of them are independent,
- with differentiation we even get differential equations for these “masters”

Perturbative components

A side remark: what are "IBP reductions" and "Laporta" anyway?

The problem is in the solving of these IBP Identities.

Practical idea (Laporta 2000): use systematically Gauss elimination.

Open questions:

How to formulate the problem in mathematical terms,

Find a solution for any problem that will work sufficiently fast.

Hints: Gauss relations between the hypergeometric functions?

Perturbative components

Is there a way to speed up the reductions? Yes, work in Mellin space! A.M.(2005)

How? Idea: perform the Mellin integration before the phase space integrations.

Basically, the effect is: $$\frac{1}{\left(p^2+\ldots f(z)\ldots\right)^C} \to \frac{1}{\left(p^2+\ldots\right)^{C+N}}$$

Therefore, one needs to perform IBP reduction over simpler propagators but one of the powers is an abstract number. Easy to generalize to several variables …

Working in Mellin space is more effective than in z-space since one works in the natural “co-ordinates” for the IBP reduction.

Properties:

- much faster reductions,
- smaller number of master integrals,
- masters satisfy difference equations in the Mellin variable N
- purely algebraic extraction of the dependence on the kinematics.

Perturbative components

Calculations in Mellin space (cont.):

1) Unlike the DIS calculations also performed in Mellin space, our method does not rely on OPE or the Optical Theorem.

Therefore, it is suitable for not-completely inclusive processes that require separate treatment of all physical cuts!

2) The N- and z-space calculations are physically completely equivalent.

However, the N-space approach produces insight about the analytical structure of the Feynman integrals, and moreover, of the solutions to the recurrence relations like the IBP identities.

Examples:

	z-space:	N-space
Solutions in z- and N-spaces in d dimensions:	$F(\ldots\epsilon\ldots; f(z))$	$F(\ldots\epsilon, N\ldots; 1)$

Perturbative components

Application in Mellin space at two loops: the NNLO coefficient functions in e^+e^-

Calculate the energy spectrum of massless quarks and gluons at two loops:

A.M., S-O Moch (2006)

$$\frac{d\sigma^{(T,L,A)}}{dz} \quad ; \quad e^+e^- \to \; q/g + X \quad ; \quad 0 \leq z \leq 1$$

Evaluated in expansion around d=4:

$$\frac{d\sigma}{dz} = \cdots + \alpha_S^2 \left(\cdots + P/\epsilon + A\epsilon^0 + B\epsilon^1 + \dots \right)$$

During the evaluation we encounter:

- 6 N-dependent Real-Real Masters → Expressed in harmonic sums with
- 5 N-dependent Real-Virtual Masters → the help of the difference equations.

The dependence on the kinematics is extracted algebraically. Only 7 integrals have to be evaluated and they are pure numbers independent of kinematics. They were derived previously in a different context:

Gehrmann-De Ridder, Gehrmann, Heinrich (2003)

Working in Mellin space minimizes the evaluation of Feynman integrals !

Perturbative components

The 3-loop time-like splitting functions (needed for NNLO evolution)

Idea: all non-singlet functions can be extracted from the $1/\epsilon$ poles at three loops in e^+e^-

$$\frac{d\sigma}{dz} = \delta(1-z) + \alpha_S \left(P^{(0)T}/\epsilon + C^{(0)T} + B^{(0)T}\epsilon \right) + \cdots + \alpha_S^3 \left(\cdots + P^{(2)T}/\epsilon + C^{(2)T} + \ldots \right)$$

But VERY hard to calculate directly at present. The only distribution know to three loops at present are the three-loops calculations in DIS: Moch, Vermaseren Vogt (2004,2005)

$$\frac{d\sigma}{dx} = \delta(1-x) + \alpha_S \left(P^{(0)S}/\epsilon + C^{(0)S} + B^{(0)S}\epsilon \right) + \cdots + \alpha_S^3 \left(\cdots + P^{(2)S}/\epsilon + C^{(2)S} + \ldots \right)$$

The structure of the two cross-sections is similar; is there a relation between the two?

Previously results only at low orders and only between the splitting functions:

LO Gribov, Lipatov (1972)

NLO Curci, Furmanski, Petronzio (1980)

We propose an analytical continuation DIS → e^+e^- A.M., S-O Moch, A. Vogt (2006)

Perturbative components

The 3-loop time like splitting functions (cont.)

The analytical continuation we propose is able to exactly predict the e^+e^- partonic cross-section at orders α_S (NLO) and α_S^2 (NNLO) for each known power of ϵ .

The continuation explores mass factorization and requires matching of:

- amplitudes (exact)
- scaling variables $\left(x \to 1/z \ ; \ Q^2 \to \ - Q^2\right)$
- proper phase-space modifications (multiplicative factor of $z^{1-2\epsilon}$)
- matching the analytical continuation of branch cuts (harder)

What happens when we apply It to 3 loops?

- All poles higher than $1/\epsilon$ are predicted correctly,
- Produces a term which does not agree with the sum rules. It is of the form

$$\sim C_F^3 p_{qq}(z) \ln^2(z) \pi^2$$

We can identify the term that causes this discrepancy on physical grounds.

Perturbative components

The 3-loop time like splitting functions (cont.)

The corrected 3-loop non-singlet prediction coincides with another one due to Dokshitzer, Marchesini and Salam (2005) for the difference between the space- and time-like functions.

Although the 3-loop splitting functions are very complicated, their difference is quite compact:

$$P^{(2),T} - P^{(2),S} = \left[\ln(z).\left(P^{(1),T} + P^{(1),S}\right)\right] \otimes P^{(0)} + \left[P^{(1),T} + P^{(1),S}\right] \otimes \left[\ln(z).P^{(0)}\right]$$

In fact it is even possible to extend the arguments of DSM to get the difference between space- and time-like non-singlet splitting functions even at 4 loops!

Work is underway:

- on the singlet components,
- independent checks/derivations,
- extend the results to 3-loop coefficient functions (Longitudinal fragmentation)

Towards b-fragmentation at NNLO

To properly predict b-quark fragmentation one has to:

- predict the spectrum of the massive b-quark at FO (NNLO)
- resum the large mass logs to NNLL with DGLAP
- fit LEP data to extract the non-perturbative fragmentation function.

$$e^+e^- : \qquad \frac{d\sigma_B}{dE} = \frac{d\sigma_b}{dE} \otimes D^{ini} \otimes D^{DGLAP} \otimes D^{\text{n.p.}}_{b\to B} \; + \; O(m^2)$$

Up to terms ~ O(m) one can predict the massive b-spectrum from purely massless calculations:

- massless coefficient functions

Rijken and van Neerven (1996)
A.M. and Sven Moch (2006)

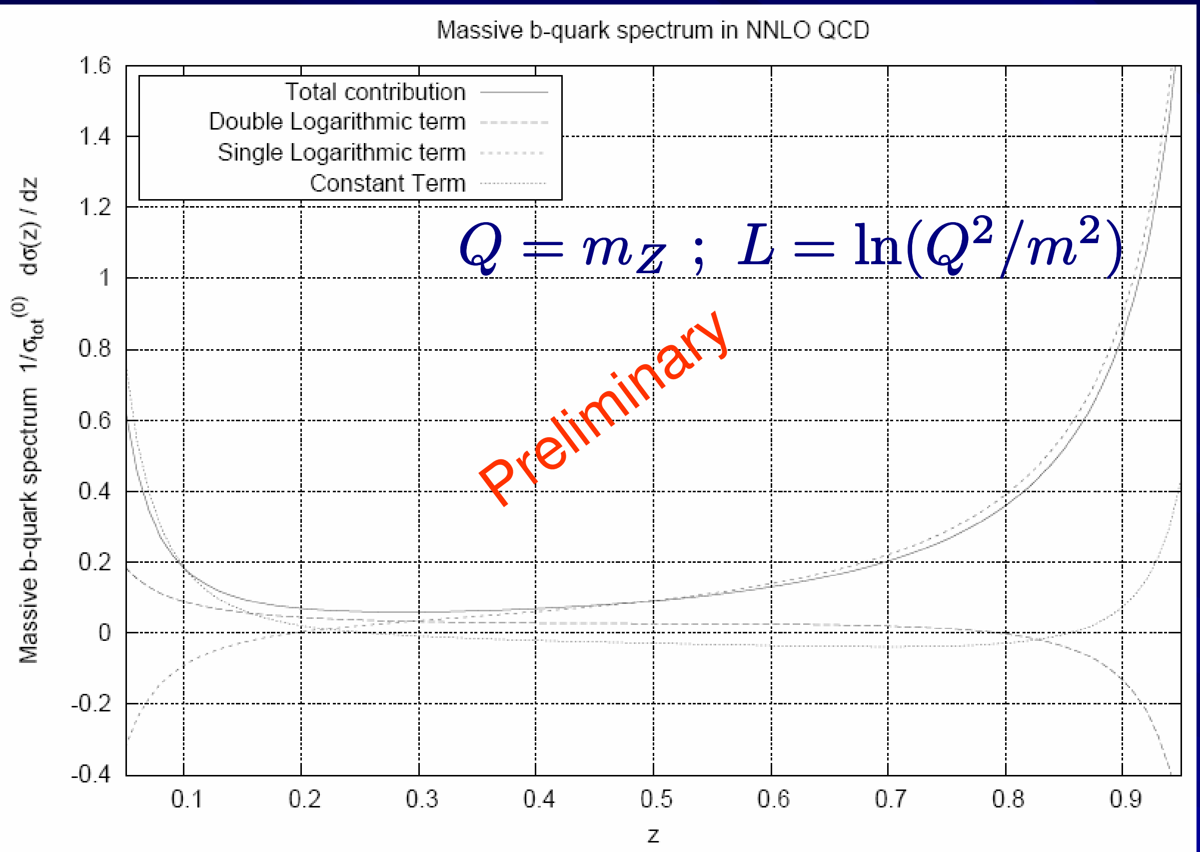
- Perturbative Fragmentation Function: Mele-Nason (1991 at NLO)

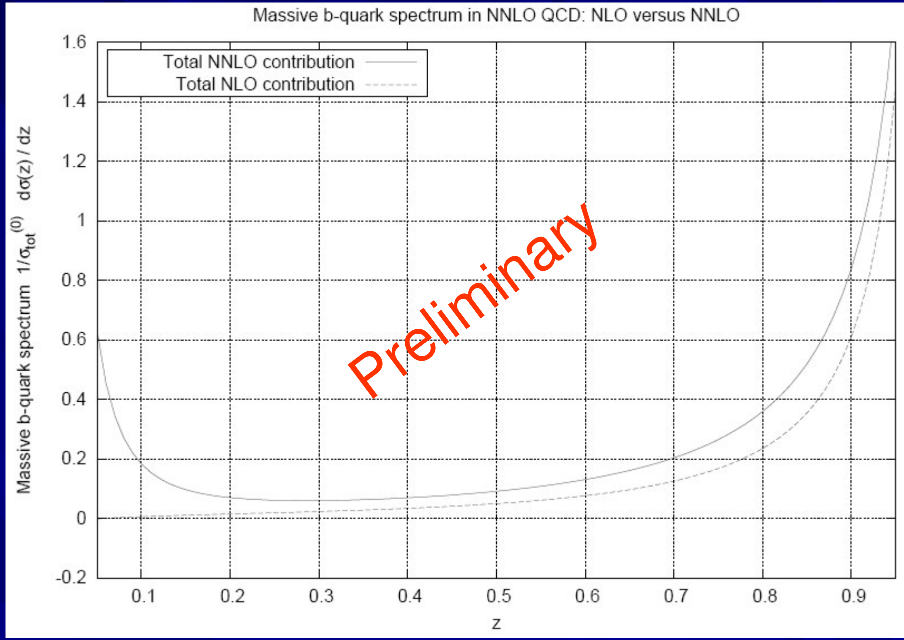
Kirill Melnikov, A.M.; A.M. (2004) at NNLO

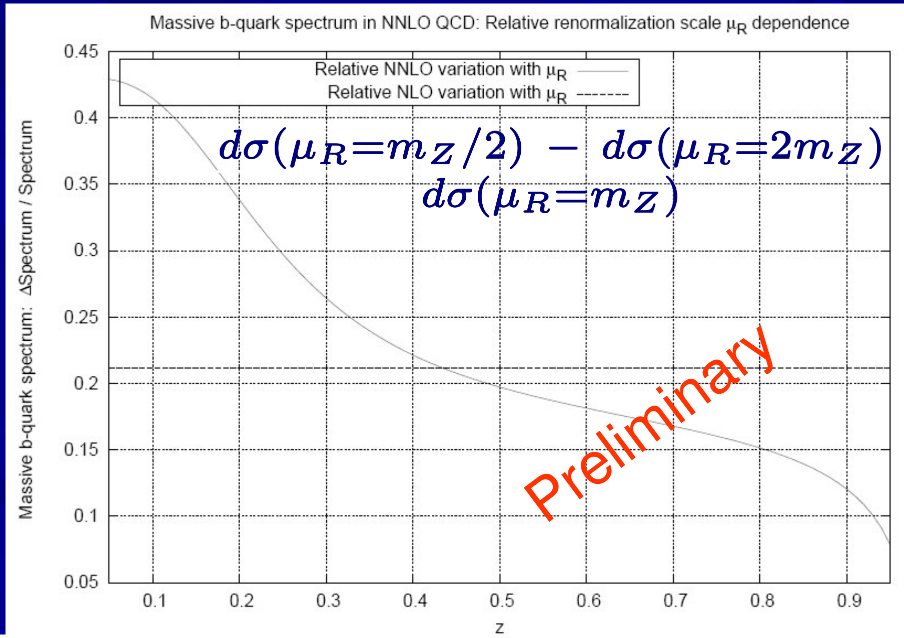
This formalism has so far been only applied to NLO and for the logarithmic terms at NNLO. Here, it is applied for a first time to predict the “constant contribution”.

Some preliminary plots:

Towards b-fragmentation at NNLO







The soft-gluon, soft "singlet" contribution enters for the first time at this order. Will improve with resummation.

Not checked yet vs the numerical results for the same observable Nason, Oleari (1999). The O(m) terms?

Summary

- There have been exciting developments towards b-fragmentation at NNLO :
- Two-loop coefficient functions in electron positron annihilation,
- New calculational method in Mellin space,
- 3-loop non-singlet time-like splitting functions,
- The perturbative heavy quark Fragmentation Function at two loops.

- Presented first application to massive b-spectrum at NNLO from massless calculations. Interesting new features!

- Expect soon results on extracted b-fragmentation function at NNLO!

Applications (especially LHC)

- P_T - distribution of b-quarks,
- Extension to charm is also possible.
- Precise top mass measurement from J/Ψ in top decay.
- b- and t-production at hadron colliders at NNLO.